

# Gouy Phase for Relativistic Quantum Particles

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Recently Gouy rotation was observed with focused non-relativistic electron vortex beams. If the electrons in vortex beams are very fast we have to take into account relativistic effects to completely describe the Gouy phase on them. Exact Hermite-Gaussian solutions to the Klein-Gordon equation for particle beams are obtained here that make explicit the 4-position of the focal point of the beam. These are Bateman-Hillion solutions with modified phase factors to take into account the rest mass of the particles. They enable a relativistic expression for the Gouy phase to be determined. It is in fact shown all the solutions are form invariant under Lorentz transformations. It is further shown for the exact solutions to correspond to those of the Schrödinger equation the relative time between the focal point and any point in the beam must be constrained to be a specific function of the relative spatial coordinates.

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*Introduction* - The Gouy phase of matter waves in the non-relativistic context have been explored firstly in [1, 2], followed by experimental realizations with Bose-Einstein condensates [3], electron vortex beams [4] and astigmatic electron matter waves using in-line holography [5]. Also, it was showed that to improve the accuracy in imaging the dynamics of free-electron Landau states the diffractive Gouy phase rotation has to be reduced [6].

Electron vortex beams recently have been theoretically and experimentally explored since they can be applied to improved electron microscopy of magnetic and biological specimens [7, 8]. Production of electron vortex beams with high-energy and orbital quantum number seems feasible [9]. The Angular Momentum and Spin-Orbit interaction in the relativistic electron vortex beams was studied in terms of the Dirac equation in [10]. The Gouy phase for this case, which was not treated in [10], is completely explained only if relativistic effects be considered and in this letter we explore these possible effects in the Gouy phase. The experimentally observed solutions for electron vortex beams with carry out Orbital Angular Momentum (OAM) could be expressed in terms of the solutions that will be obtained here. In order to avoid additional complications we do not take into account the spin of particle and we will solve here the Klein-Gordon equation.

Bateman [11] discovered a class of exact solutions to the linear wave equation over a hundred years ago. Hillion [12, 13] later complexified these solutions for application to wave packet and wave beam problems. We present exact Bateman-Hillion solutions to the Klein-Gordon equation for the wave function  $\Psi(x_\mu)$  in Hermite-Gaussian beams where  $x_\mu$  denotes position in Minkowski space and  $\mu = 0, 1, 2, 3$ . Here we characterize the quantum dynamics of a relativistic particle enabling us to better understand the quantum behavior of electrons in high velocities, for example in relativistic electron vortex. As

a consequence of the relativistic effects the Gouy phase for the matter waves has a different expression from the non-relativistic counterpart that must be taken into account, especially, when we focus on a relativistic particle beam. Also, we present a method for using these solutions to calculate the properties of beams for continuous wave sources.

The origin of the coordinate system for a beam is usually at the center of the focal point. It follows the spatial coordinates  $x_i^r (i = 1, 2, 3)$  of this point are zeroed out but translating the beam will make them explicit. For relativistic solutions, it must be recognized  $x_i^r$  is part of a 4-vector such that the 4-potential is also dependent on the time coordinate  $x_0^r$ .

The fact  $\Psi$  depends on two 4-position vectors creates a problem familiar from the treatment of two interacting relativistic particles [14, 15] that the field cannot evolve in two independent time coordinates. The known solution to be applied here is to use a Dirac delta function  $\delta[f(\xi_\mu)]$  to impose a relationship  $f(\xi_\mu) = 0$  between the relative coordinates  $\xi_\mu = x_\mu - x_\mu^r$ . In classical electrodynamics, this idea leads to the derivation of the Lienard-Wiechert potentials [16] for the field experienced at one point owing to the presence of a point charge at another. The delta function notation for eliminating the relative time is also used in quantum electrodynamics [17].

For non-relativistic beams the wave function  $\Psi$  can also be calculated from the Schrödinger equation [1]. Solutions to the Schrödinger equation are harmonic in time but  $|\Psi|$  is independent of time. It is usual therefore to normalize  $\Psi$  in a 3-dimensional constraint space rather than over all Minkowski space. For the exact solutions to be developed in this letter  $|\Psi|$  does depend on time. The intent though is still to normalize them in a 3-dimensional constraint space using the  $\delta[f(\xi_\mu)]$  condition to define it.

*Hermite-Gaussian Beams* - Consider a beam of particles each having a rest mass  $m_0$ , a 4-position  $x_\mu = (x_i, t)$

and a 4-momentum  $p_\mu = (p_i, E)$ . The Klein-Gordon equation for the wave function  $\Psi(x_\mu)$  representing each of the particles in Minkowski space can be expressed as

$$(\hat{E}^2 + c^2 \hat{p}_i^2) \Psi = m_0 c^2 \Psi \quad (1)$$

where

$$\hat{p}_i = \frac{i}{\hbar} \frac{\partial}{\partial x_i}, \quad \hat{E} = -\frac{i}{\hbar} \frac{\partial}{\partial t} \quad (2)$$

are the momentum and energy operators,  $\hbar$  is Planck's constant divided by  $2\pi$  and  $c$  is the velocity of light.

Here we will find an exact solutions  $\Psi_{mn}$  to the Klein-Gordon equation (1) for Hermite-Gaussian beams moving in the  $x_3$ -direction. It will be assumed this takes the Bateman inspired form

$$\Psi_{mn} = \Phi_{mn}(\xi_1, \xi_2, \xi_3 + c\tau) \exp[i(k_3 x_3 - \omega t)], \quad (3)$$

where

$$\xi_i = x_i - x_i^r, \quad \tau = t - t^r \quad (4)$$

gives the position of each point  $x_\mu$  relative to the center of the focal point of the beam  $x_\mu^r$ ,  $k_3$  is the wave vector component along the direction of the beam,  $\omega$  is the angular frequency and  $\Phi_{mn}$  are scalar functions. The positive integers  $m$  and  $n$  indicate the mode of the beam.

Inserting eq. (3) into the Klein-Gordon equation (1) gives

$$\left[ \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + 2i \left( k_3 \frac{\partial}{\partial x_3} + \frac{\omega}{c^2} \frac{\partial}{\partial t} \right) \right] \Phi_{mn} = 0, \quad (5)$$

having spotted

$$\left( \frac{\partial^2}{\partial x_3^2} - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} \right) \Phi_{mn} = 0, \quad (6)$$

owing to the dependence of  $\Phi_{mn}$  on  $\xi_3$  and  $\tau$  in the linear combination  $\xi_3 + c\tau$ .

Equation (5) is analogous to the paraxial wave equation

$$\frac{\partial^2 \Phi_{mn}^P}{\partial x_1^2} + \frac{\partial^2 \Phi_{mn}^P}{\partial x_2^2} + 2ik_3 \frac{\partial \Phi_{mn}^P}{\partial x_3} = 0, \quad (7)$$

where the role of  $\xi_3$  in  $\Phi^P(\xi_1, \xi_2, \xi_3)$  is replaced by  $\xi_3 + c\tau$  in  $\Phi(\xi_1, \xi_2, \xi_3 + c\tau)$ . It can therefore be solved analogously [18] to give

$$\Phi_{mn} = \frac{C_{mn} w_0}{w} H_m \left( \frac{\sqrt{2} \xi_1}{w} \right) H_n \left( \frac{\sqrt{2} \xi_2}{w} \right) \times \quad (8)$$

$$\exp \left[ \frac{i(k_3 + \frac{\omega}{c})(\xi_1^2 + \xi_2^2)}{\xi_3 + c\tau - 2ib} - ig_{mn} \right], \quad (9)$$

where  $H_m$  and  $H_n$  are Hermite polynomials,

$$b = \frac{1}{2} \left( k_3 + \frac{\omega}{c} \right) w_0^2, \quad (10)$$

$$w(\xi_3, \tau) = w_0 \sqrt{1 + \left( \frac{\xi_3 + c\tau}{2b} \right)^2}, \quad (11)$$

is the beam radius,  $w_0 = w(0, 0)$  is the beam waist and

$$g_{mn}(\xi_3, \tau) = (1 + m + n) \arctan \left( \frac{\xi_3 + c\tau}{2b} \right), \quad (12)$$

is the Gouy phase of a relativistic quantum particle. We observe that it depends of the longitudinal direction  $x_3$  as the non-relativistic case but also it depends of the time and the speed of light. The Gouy phase is a necessary feature of our solutions that are relativistic and can be normalized. We observe that the relativistic effect in the Gouy phase can be negligible only if the evolution occur in a scale less than 1 ns and the longitudinal distance is large than 1 m.

It is proposed the normalizing constant  $C_{mn}$  in  $\Phi_{mn}$  can be determined from the condition

$$\int_{-\infty}^{+\infty} |\Psi_{mn}|^2 \delta[f(\xi_\mu)] d^4 \xi = 1, \quad (13)$$

where  $d^4 \xi = d\xi_1 d\xi_2 d\xi_3 d\tau$  and  $f(\xi_\mu)$  is to be determined. For physical interpretation, it is clear a physical system cannot evolve in the two independent times  $t$  and  $\tau$ . The intent of the  $f(\xi_\mu) = 0$  constraint condition is therefore to eliminate the relative time in terms of the relative spatial coordinates.

*Lorentz Transformations* - The wave function  $\Psi_{mn}(x_\mu)$  has been determined in eq. (8) to be an exact solution of the Klein-Gordon eq. (1) for a particle in a beam. The task ahead is to confirm these solutions are form preserving under Lorentz transformations.

A 4-vector  $q_\mu$  is relativistic if it preserves its form under the Lorentz transformation equations:

$$q'_i = q_i + \gamma \frac{v_i}{c} \left( \frac{\gamma}{1 + \gamma} \frac{v_j q_j}{c} - q_0 \right), \quad (14)$$

$$q'_0 = \gamma \left( q_0 - \frac{v_j q_j}{c} \right), \quad (15)$$

(see ref. [16]) where  $v_i$  is the relative velocity between any two inertial reference frames and  $\gamma = (1 - v^2)^{-1/2}$ . For current purposes  $q_\mu$  belongs to the set of position  $x_\mu$ , relative position  $\xi_\mu$ , wave vector  $k_\mu$  and 4-momentum  $p_\mu$ .

To confirm the Hermite-Gaussian beam solutions are fully relativistic it will be necessary to investigate the Lorentz transformation of number of different quantities including the phase factor, the Gaussian function, the Hermite functions, and Gouy phase. For brevity, the analysis will be limited to the case of an observer that is moving parallel to the axis of the beam.

The product  $k_\mu x_\mu$  is Lorentz covariant implying

$$k'_\mu x'_\mu = k_\mu x_\mu. \quad (16)$$

The numerator and denominator in the Gaussian component of eq. (8) can be transformed separately to give

$$\left(k'_3 + \frac{\omega'}{c}\right)(\xi_1'^2 + \xi_2'^2) = \sqrt{\frac{c-v}{c+v}} \left(k_3 + \frac{\omega}{c}\right)(\xi_1^2 + \xi_2^2), \quad (17)$$

and

$$\xi_3' + c\tau' - 2ib' = \sqrt{\frac{c-v}{c+v}}(\xi_3 + c\tau - 2ib), \quad (18)$$

having determined

$$b' = \sqrt{\frac{c-v}{c+v}}b, \quad (19)$$

from eq. (10) assuming the radius  $w_0$  is a Lorentz invariant scalar. Putting these results together leads to

$$\frac{\left(k'_3 + \frac{\omega'}{c}\right)(\xi_1'^2 + \xi_2'^2)}{\xi_3' + c\tau' - 2ib'} = \frac{\left(k_3 + \frac{\omega}{c}\right)(\xi_1^2 + \xi_2^2)}{\xi_3 + c\tau - 2ib}. \quad (20)$$

Eqs. (17) through (20) can now be used to transform eq. (8) into  $\Phi'_{mn}$  is equal to

$$\frac{C_{mn}w_0}{w'} H_m \left( \frac{\sqrt{2}\xi_1'}{w'} \right) H_n \left( \frac{\sqrt{2}\xi_2'}{w'} \right) \times \quad (21)$$

$$\exp \left[ \imath \frac{\left(k'_3 + \frac{\omega'}{c}\right)(\xi_1'^2 + \xi_2'^2)}{\xi_3' + c\tau' - 2ib'} - \imath g'_{mn} \right], \quad (22)$$

where

$$w' = w_0 \sqrt{1 + \left( \frac{\xi_3' + c\tau'}{2b'} \right)^2} = w_0 \sqrt{1 + \left( \frac{\xi_3 + c\tau}{2b} \right)^2}, \quad (23)$$

$$\frac{g'_{mn}}{(1+m+n)} = \arctan \left( \frac{\xi_3' + c\tau'}{2b'} \right) = \arctan \left( \frac{\xi_3 + c\tau}{2b} \right), \quad (24)$$

and  $C_{mn}$  is a Lorentz invariant scalar.

It follows from taking stock of all of these results that eq. (3) can be rewritten as

$$\Psi'_{mn} = \Phi_{mn}(\xi_1', \xi_2', \xi_3' + c\tau') \exp(\imath k'_3 x'_3 - \imath \omega' t'). \quad (25)$$

On comparing eqs. (3) and (25) it is concluded  $\Psi_{mn}$  is form invariant under Lorentz transformations and therefore fully relativistic.

*Correspondence to the Schrödinger Equation* - The objective here is to determine the form of the constraint condition  $f(\xi_\mu) = 0$  in eq. (13) from the principle that exact solutions of the Klein-Gordon equation should correspond to solutions of the Schrödinger equation in the non-relativistic limit. The Schrödinger equation takes the form

$$\frac{\partial^2 \Psi_{mn}^S}{\partial x_1^2} + \frac{\partial^2 \Psi_{mn}^S}{\partial x_2^2} + \frac{\partial^2 \Psi_{mn}^S}{\partial x_3^2} + 2\imath \frac{m}{\hbar} \frac{\partial \Psi_{mn}^S}{\partial t} = 0. \quad (26)$$

For paraxial beams, the solution  $\Psi_{mn}^S$  may be assumed to take the form

$$\Psi_{mn}^S = \Phi_{mn}^S(\xi_1, \xi_2, \tau) \exp \left[ \frac{\imath}{\hbar} (p_3 x_3 - E_s t) \right], \quad (27)$$

where

$$E_s = \frac{p_3^2}{2m_0}, \quad (28)$$

is non-relativistic kinetic energy. Inserting eq. (27) into eq. (26) gives

$$\frac{\partial^2 \Phi_{mn}^S}{\partial x_1^2} + \frac{\partial^2 \Phi_{mn}^S}{\partial x_2^2} + 2\imath \frac{m}{\hbar} \frac{\partial \Phi_{mn}^S}{\partial t} = 0. \quad (29)$$

Equation (29) is analogous to eq. (5) where the role of  $\tau$  in  $\Phi^S(\xi_1, \xi_2, \tau)$  replaces  $\xi_3 + c\tau$  in  $\Phi(\xi_1, \xi_2, \xi_3 + c\tau)$ .

The solution to eq. (29) is

$$\Phi_{mn}^S = \frac{C_{mn}w_0}{w^S} H_m \left( \frac{\sqrt{2}\xi_1}{w^S} \right) H_n \left( \frac{\sqrt{2}\xi_2}{w^S} \right) \times \quad (30)$$

$$\exp \left[ -\frac{m_0(\xi_1^2 + \xi_2^2)}{m_0 w_0^2 + 2\imath \hbar \tau} - \imath g_{mn}^S \right], \quad (31)$$

where

$$w^S(\tau) = w_0 \sqrt{1 + \left( \frac{\hbar \tau}{m_0 w_0^2} \right)^2}, \quad (32)$$

is the beam radius and

$$g_{mn}(\tau) = (1+m+n) \arctan \left( \frac{\hbar \tau}{m_0 w_0^2} \right), \quad (33)$$

is the non-relativistic Gouy phase for matter waves.

It can now be shown that the Schrödinger and exact Klein-Gordon beam solutions are related to each other through the expression

$$\Phi_{mn}^S = \int \Phi_{mn} \delta(\xi_3 - u_3 \tau) dt, \quad (34)$$

in the non-relativistic limit. This result is most easily demonstrated for the case of a Gaussian beam

$$\Phi_{00} = \frac{C_{00}b}{b + \imath \frac{1}{2}(\xi_3 + c\tau)} \exp \left[ \frac{\imath (k_3 + \frac{\omega}{c})(\xi_1^2 + \xi_2^2)}{\xi_3 + c\tau - \imath 2b} \right]. \quad (35)$$

On setting,

$$k_3 = \frac{m_0 u_3 \gamma}{\hbar}, \quad \omega = \frac{m_0 c^2 \gamma}{\hbar}, \quad (36)$$

eq. (34) evaluates to

$$\Phi_{00}^S = \frac{C_{00}m_0 w_0^2}{m_0 w_0^2 + 2\imath \hbar \tau} \exp \left[ \frac{-m_0(\xi_1^2 + \xi_2^2)}{m_0 w_0^2 + 2\imath \hbar \tau} \right], \quad (37)$$

having assumed  $\gamma \simeq 1$ . The calculation for all the higher order modes follows similarly.

It has been shown that in order for exact Bateman-Hillion solutions of the Klein-Gordon equation for Hermite-Gaussian beams of matter waves to correspond to solutions of the Schrödinger equation in the non-relativistic limit, they must be restricted to the constraint space

$$f(\xi_\mu) = \xi_3 - u_3\tau = 0. \quad (38)$$

This result is straightforward to interpret for particles large enough to have classical properties since the expression  $\xi_3 - u_3\tau = 0$  describes the trajectory of a classical free particle along the axis of the beam. It is unexpected that smaller quantum particles also appear to be confined to this constraint space.

*Discussion* - Exact solutions have been derived to the Klein-Gordon equation for matter waves Hermite-Gaussian beams using Bateman-Hillion functions. The solutions have been shown to preserve their form under Lorentz transformations. These exact solutions are not time-harmonic but it has been found they can be used to produce results comparable to time-harmonic solutions providing they are normalized and interpreted in a 3-dimensional constraint space. The guiding principle is time-harmonic and Bateman-Hillion solutions can only be compared if the calculations are performed in spaces that have the same number of dimensions.

It has been shown that for Klein-Gordon and Schrödinger beams to be in correspondence in the non-relativistic limit, the Klein-Gordon solution must be restricted to the  $\delta(\xi_3 - u_3\tau)$  constraint space. The constraint equation  $\xi_3 - u_3\tau = 0$  describes the trajectory of a classical particle. In this sense, it is intuitive that particles large enough to exhibit classical properties would belong to this constraint space but surprising that smaller quantum particles also appear to be restricted to it. When the Gouy phase of matter waves was obtained in [1], the constraint equation  $\xi_3 - u_3\tau = 0$  was used to transform the Schrödinger equation analogous to paraxial equation for which the propagation direction of a quantum particle is said to be classical. As the energy associated with the momentum of the particles in the propagation direction is very high to include the relativistic effects we can consider, as in [1], a classical movement in this direction which makes the Gouy phase be a function of propagation direction and the relativistic effect appear in the time coordinate, see eq. (12). If we do not consider that the momentum of the particles in the propagation direction is high we have the non-relativistic Schrödinger equation that is different from the paraxial equation but still the Gouy phase is present in the solutions of a free particle as a property of the wave behavior. However, it is a time dependent function instead of a function dependent of the propagation direction.

In conclusion, we have shown that the Gouy phase of

relativistic quantum particle can be obtained by transforming the Klein-Gordon equation to an analogue of paraxial equation which provides normalized and Lorentz invariant solutions. The relativistic Hermite-Gaussian solutions contain Orbital Angular Momentum (OAM) and form a complete basis. These results can therefore be applied to treat relativistic electron vortex beams. It is anticipated though for strongly converging or diverging beams that  $\delta(\xi_3 - u_3\tau)$  would need to be replaced to a form such as  $\delta(|\xi_i| - |u_i|\tau)$  for better correspondence to the trajectories of classical particles in the case  $m_0$  is large.

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- [1] I. G. da Paz, M. C. Nemes, S. Padua, C. H. Monken, and J.G. Peixoto de Faria, Phys. Lett. A **374**, 1660 (2010).
  - [2] I. G. da Paz, P. L. Saldanha, M. C. Nemes, and J. G. Peixoto de Faria, New Journal of Phys. **13**, 125005 (2011).
  - [3] A. Hansen, J. T. Schultz, and N. P. Bigelow, Conference on Coherence and Quantum Optics Rochester (New York, United States, 2013); J. T. Schultz, A. Hansen, and N. P. Bigelow, Opt. Lett. **39**, 4271 (2014).
  - [4] G. Guzzinati, P. Schattschneider, K. Y. Bliokh, F. Nori, and J. Verbeeck, Phys. Rev. Lett. **110**, 093601 (2013).
  - [5] T. C. Petersen, D. M. Paganin, M. Weyland, T. P. Simula, S. A. Eastwood, and M. J. Morgan, Phys. Rev. A **88**, 043803 (2013).
  - [6] P. Schattschneider, T. Schachinger, M. Stöger-Pollach, S. Löffler, A. Steiger-Thirsfeld, K. Y. Bliokh, and F. Nori, Nature Communications **5**, 1 (2014).
  - [7] J. B. McMorran, A. Agrawal, I. M. Anderson, A. A. Herzog, H. J. Lezec, J. J. McClellan, and J. Unguris, Science **331**, 192 (2011).
  - [8] J. Verbeeck, H. Tian, and P. Schattschneider, Nature (London) **467**, 301 (2010); P. Schattschneider and J. Verbeeck, Ultramicroscopy **111**, 1461 (2011); J. Verbeeck, P. Schattschneider, S. Lazar, M. Stöger-Pollach, S. Löffler, A. Steiger-Thirsfeld, and G. Van Tendeloo, Appl. Phys. Lett. **99**, 203109 (2011); S. Lloyd, M. Babiker, and J. Yuan, Phys. Rev. Lett. **108**, 074802 (2012).
  - [9] I. P. Ivanov, Phys. Rev. D **83**, 093001 (2011).
  - [10] K. Y. Bliokh, M. R. Dennis, and F. Nori, Phys. Rev. Lett. **107**, 174802 (2011).
  - [11] H. Bateman, Proc. London Math. Soc. **8**, 223 (1910).
  - [12] P. Hillion, J. Math. Phys. **33**, 2749 (1992).
  - [13] A. P. Kiselev, A. B. Plachenov, and P. Chamorro-Posada, Phys. Rev. A **85**, 043835 (2012).
  - [14] A. Komar, Phys. Rev. D **18**, 1887 (1978).
  - [15] H. W. Crater and P. Van Alstine, Phys. Rev. D **36**, 3007 (1987).
  - [16] M. Saleem and M. Rafique, *Special Relativity Applications to Particle Physics and the Classical Theory of Fields* (Ellis Horwood, 1992).
  - [17] R.P. Feynman, *Quantum Electrodynamics* (Addison Wesley, 1962).
  - [18] A. E. Siegman, *Lasers* (University Science Books, 1986).